LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	60	63	80	rVB	149657	238053	1.77%	0.375%
2	4.569	279	286	295	rBV	216708	322813	2.40%	0.509%
3	5.016	355	362	383	rBV	3739170	5431053	40.43%	8.565%
4	6.575	616	627	642	rBV	3713764	5763651	42.90%	9.089%
5	7.357	753	760	769	rBV	776585	1197632	8.91%	1.889%
6	8.504	948	955	967	rBV	2307250	3763012	28.01%	5.934%
7	9.087	1048	1054	1061	rBV	92449	146664	1.09%	0.231%
8	10.116	1221	1229	1238	rBV	951494	1605584	11.95%	2.532%
9	10.875	1352	1358	1371	rBV	152335	312336	2.32%	0.493%
10	12.628	1648	1656	1671	rBV	5618405	8393051	62.47%	13.236%
11	14.022	1886	1893	1901	rBV	1525359	2271623	16.91%	3.582%
12	15.527	2143	2149	2171	rBV	5109237	7796364	58.03%	12.295%
13	16.786	2356	2363	2374	rBV	2004761	2850709	21.22%	4.496%
14	17.721	2517	2522	2536	rBV	786053	1220244	9.08%	1.924%
15	19.021	2739	2743	2755	rBV	367010	596555	4.44%	0.941%
16	19.457	2811	2817	2825	rBV	10572441	13434737	100.00%	21.186%
17	20.762	3034	3039	3051	rBV	1090761	1737405	12.93%	2.740%
18	21.027	3079	3084	3090	rBV	2384411	3183438	23.70%	5.020%
19	21.756	3205	3208	3209	rBV	125910	144672	1.08%	0.228%
20	23.721	3535	3542	3560	rVB	1272943	3002652	22.35%	4.735%

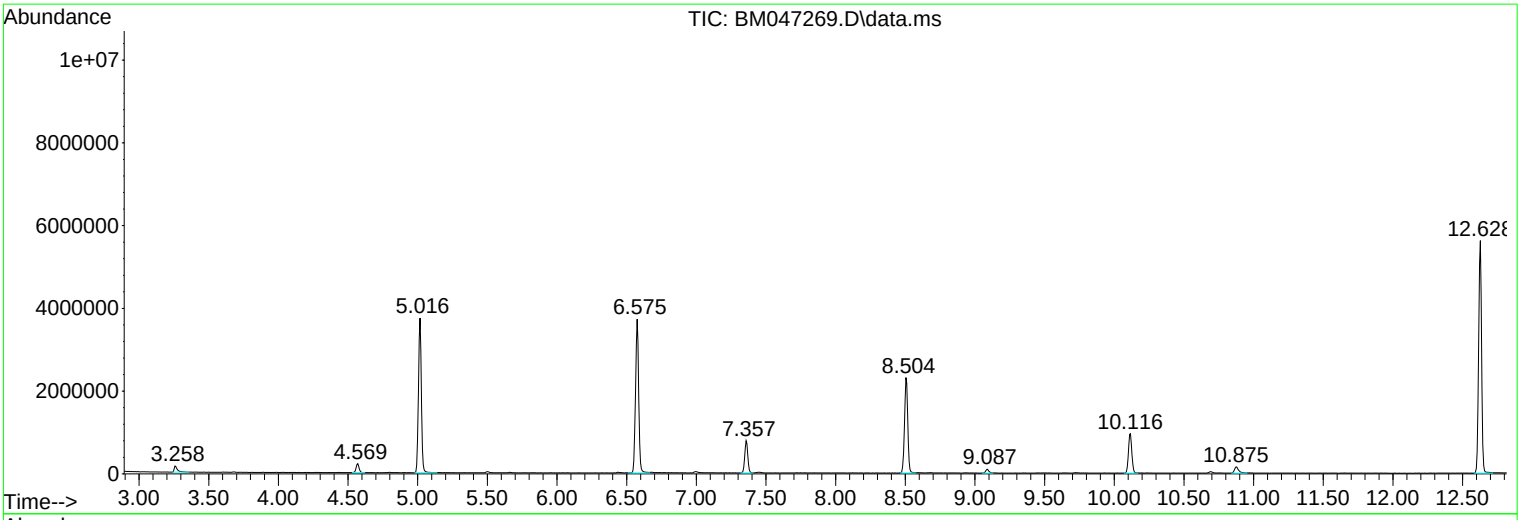
Sum of corrected areas: 63412248

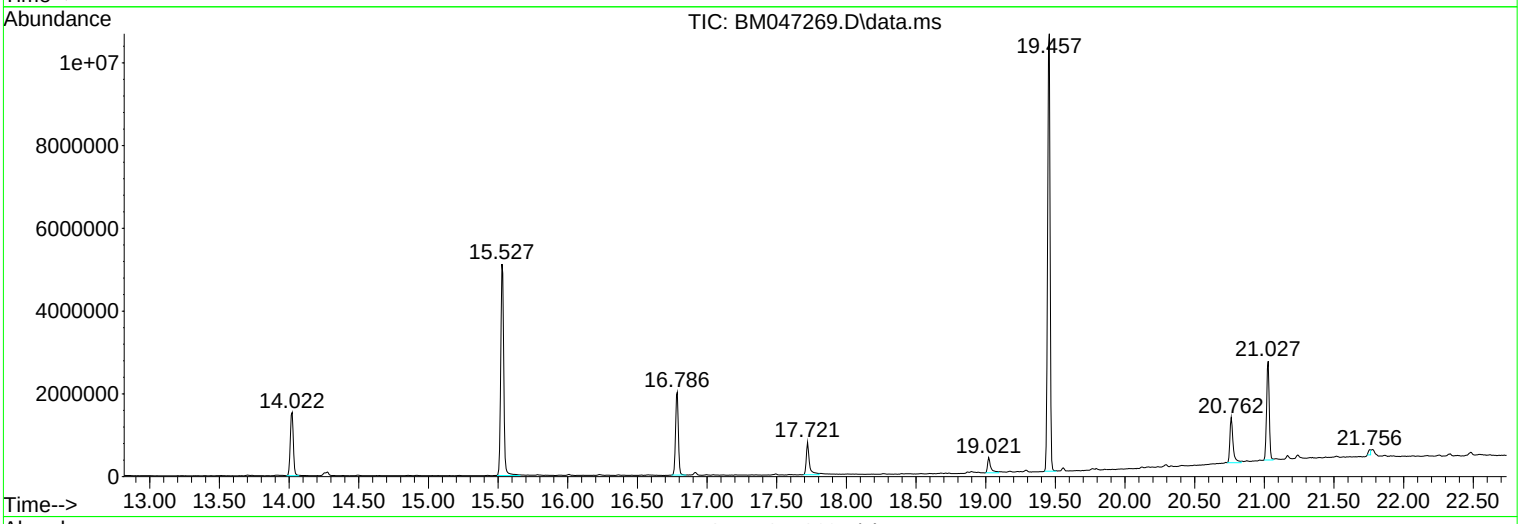
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

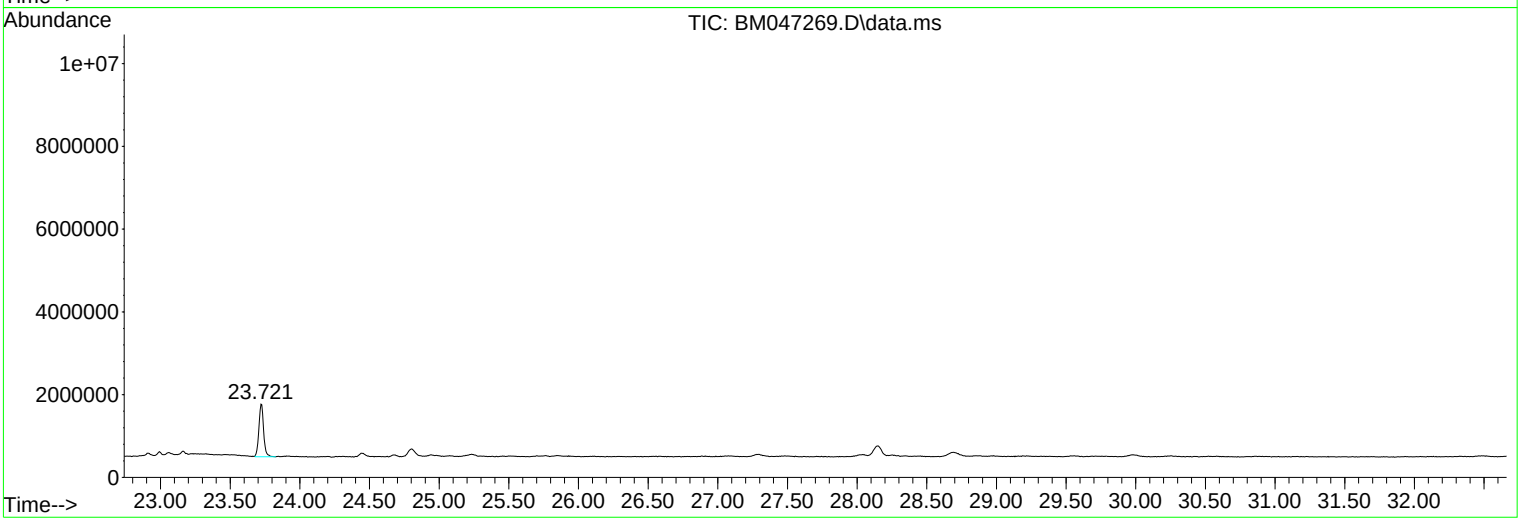
Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

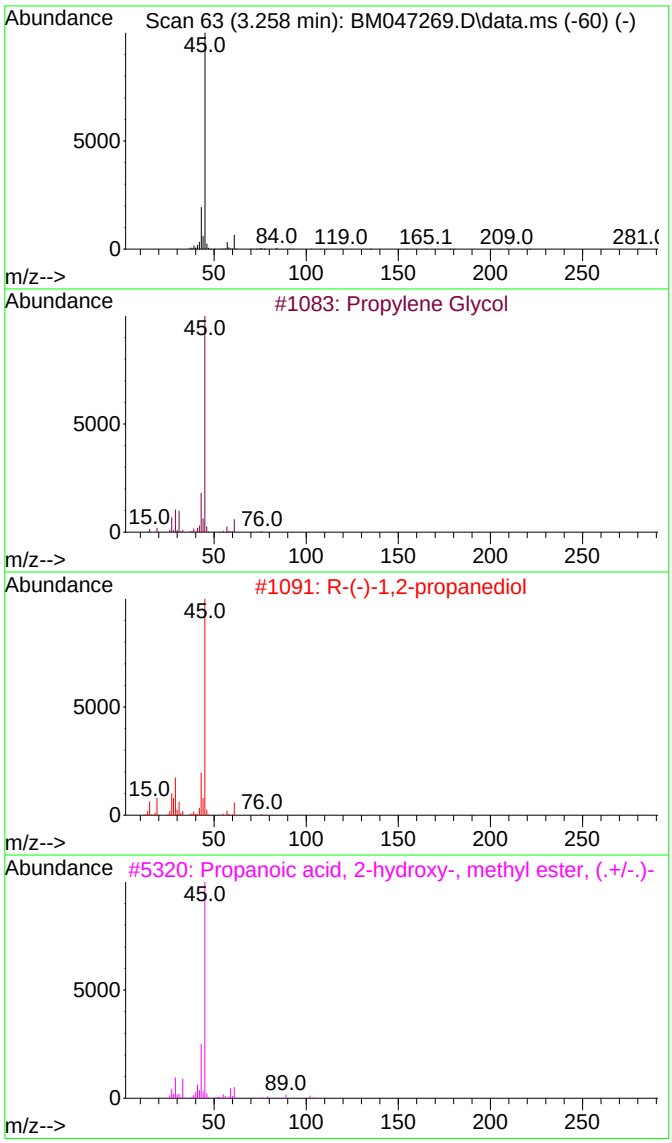
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

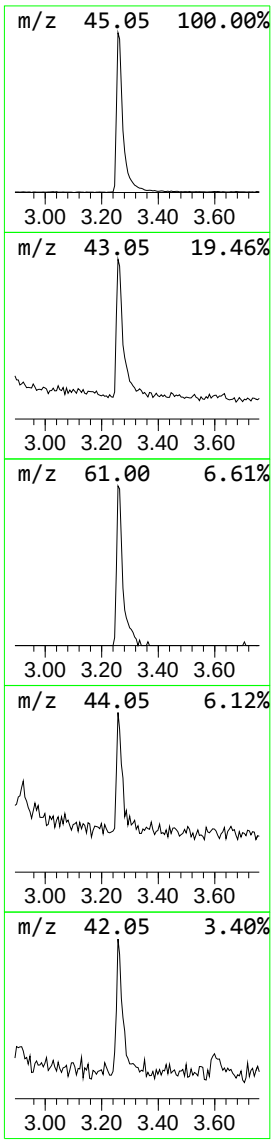
****

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	3.98 ng	238053	1,4-Dichlorobenzene-d4	7.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	39
5	2-Pentanol	88	C5H12O	006032-29-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

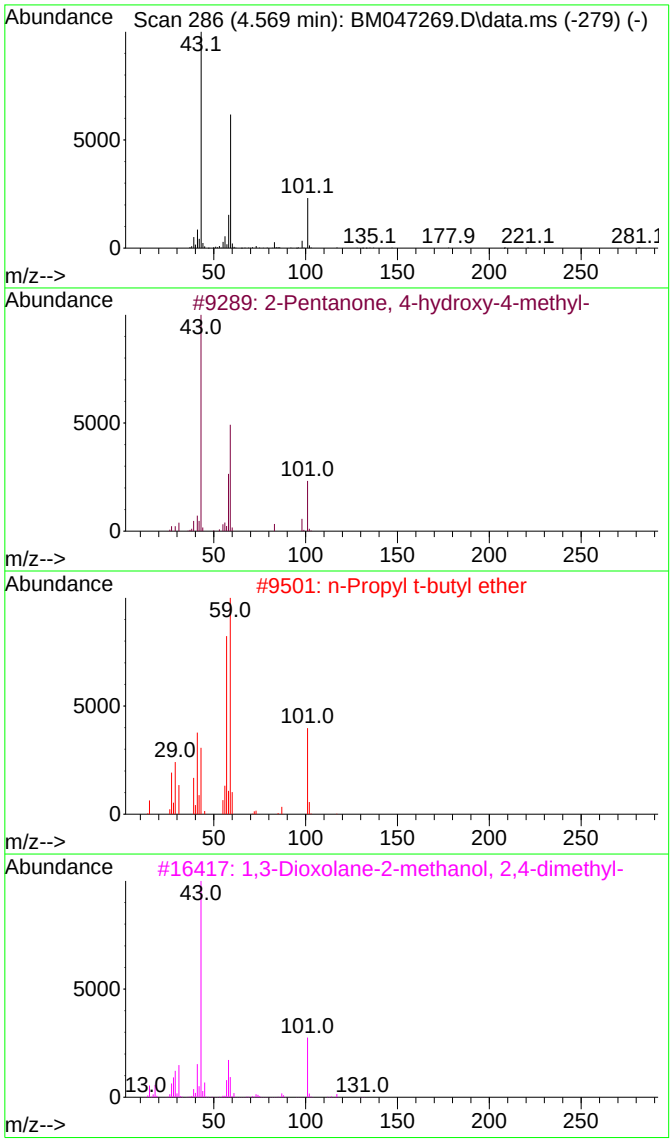
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

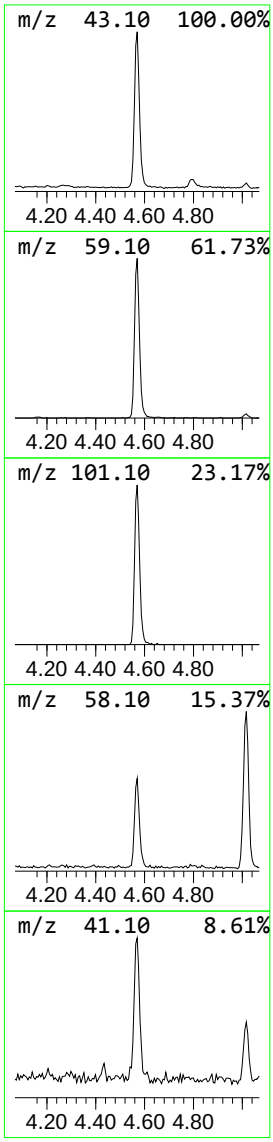
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	5.39 ng	322813	1,4-Dichlorobenzene-d4	7.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Tetraglyme	222	C10H22O5	000143-24-8	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

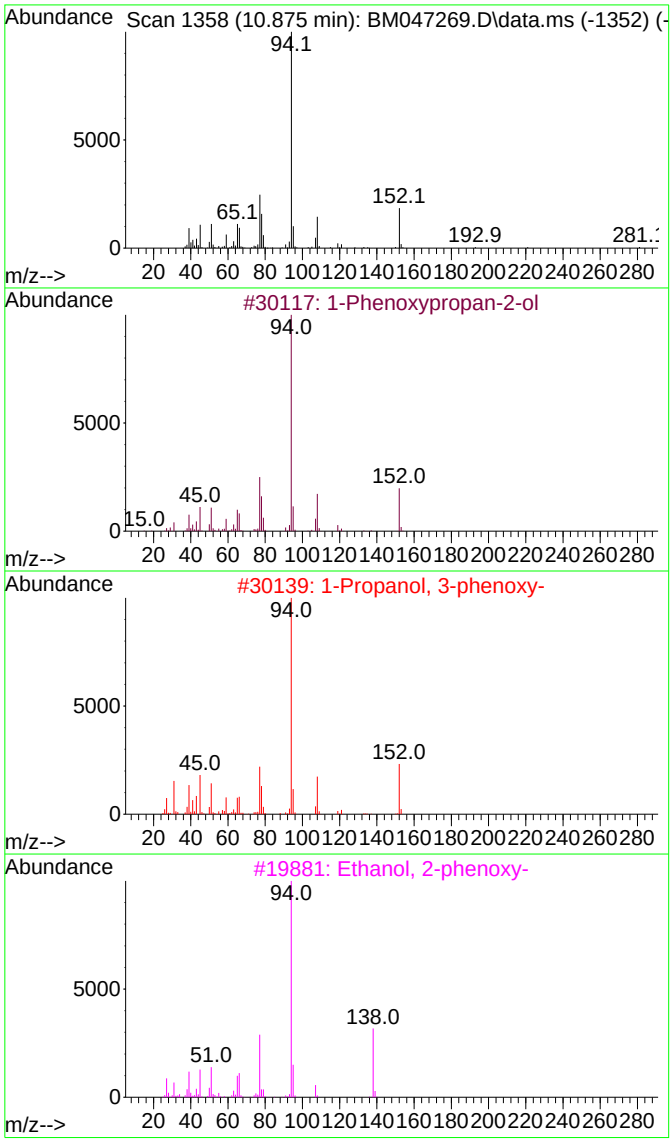
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

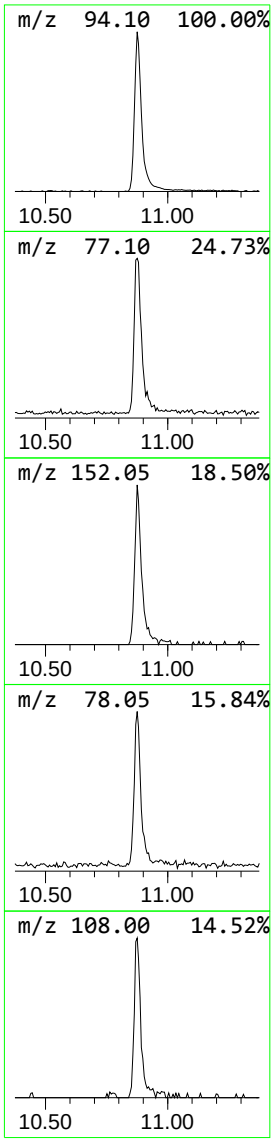
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	3.89 ng	312336	Naphthalene-d8	10.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	Acetic acid, chloro-, phenyl ester	170	C8H7ClO2	000620-73-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

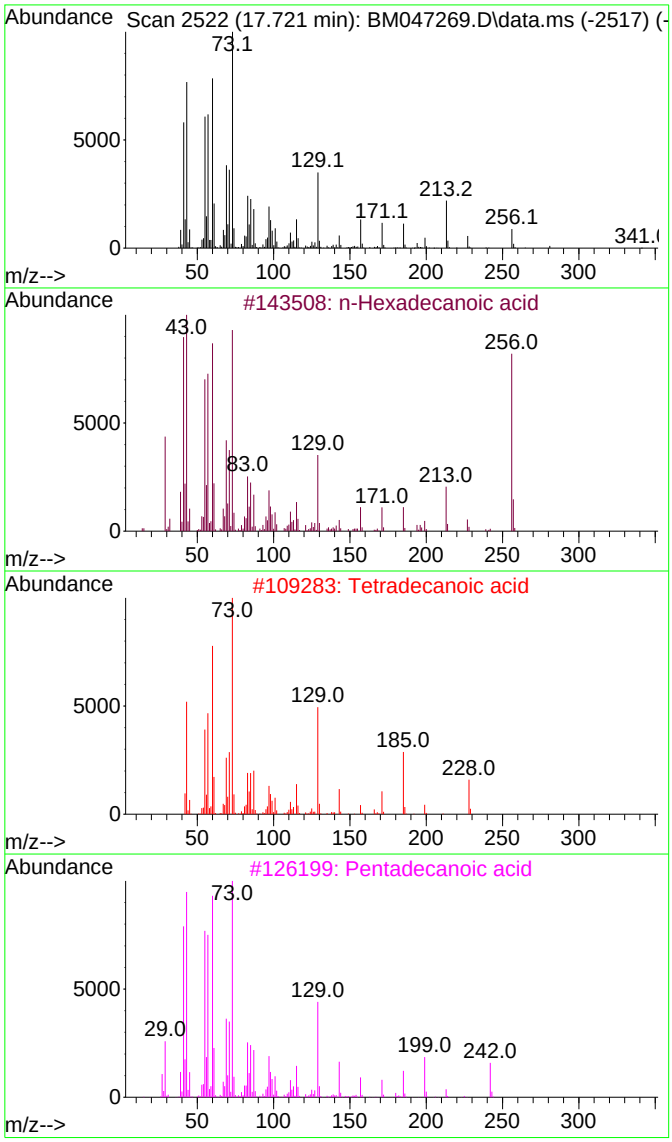
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

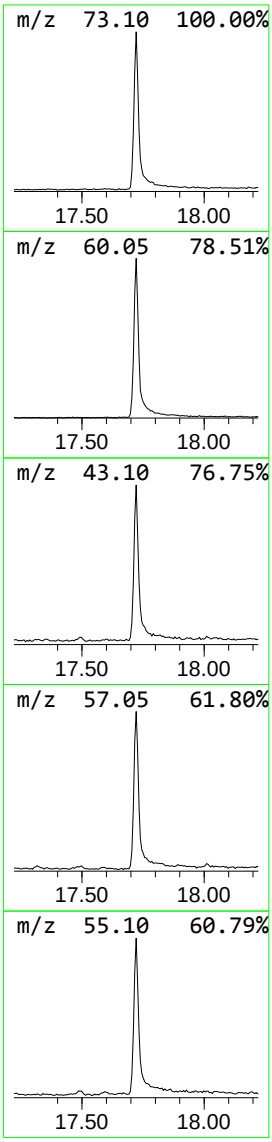
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	8.56 ng	1220240	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

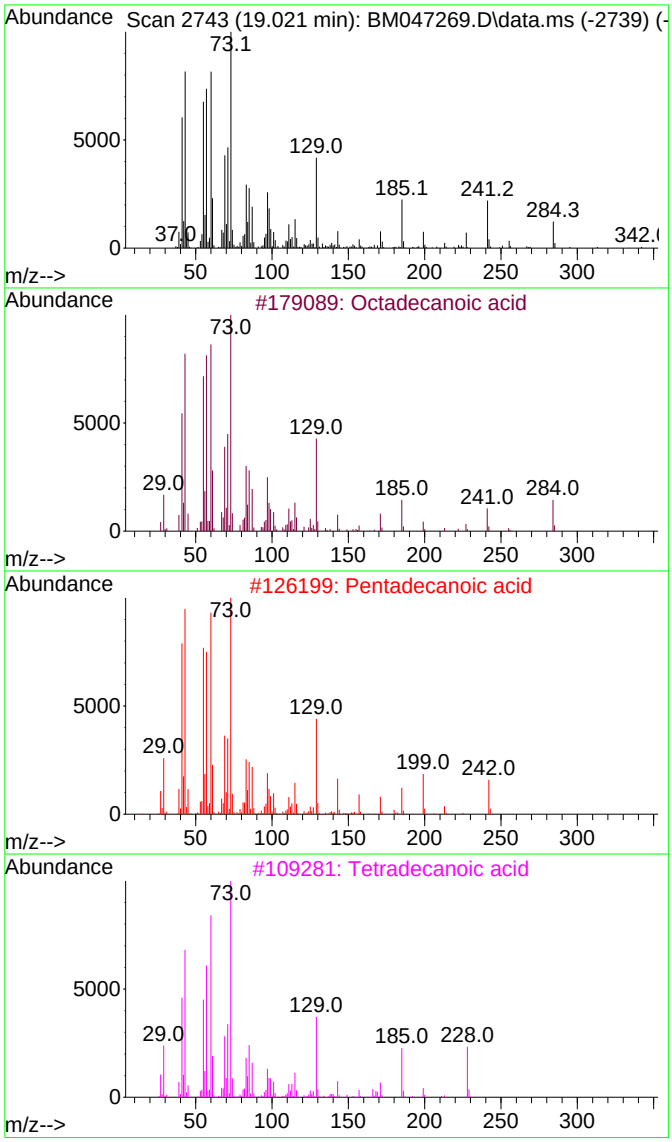
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

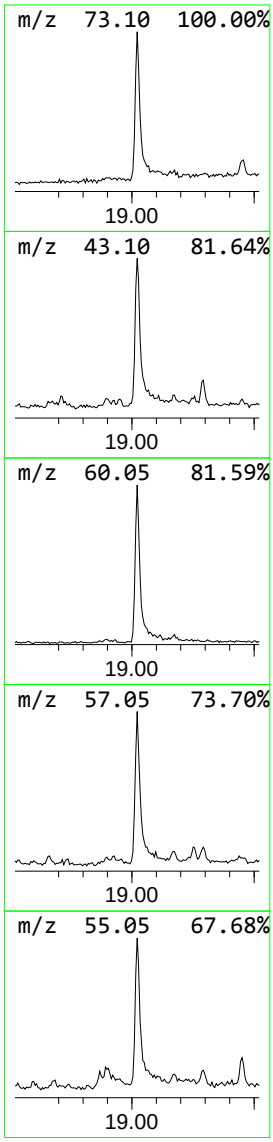
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	3.75 ng	596555	Chrysene-d12	21.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

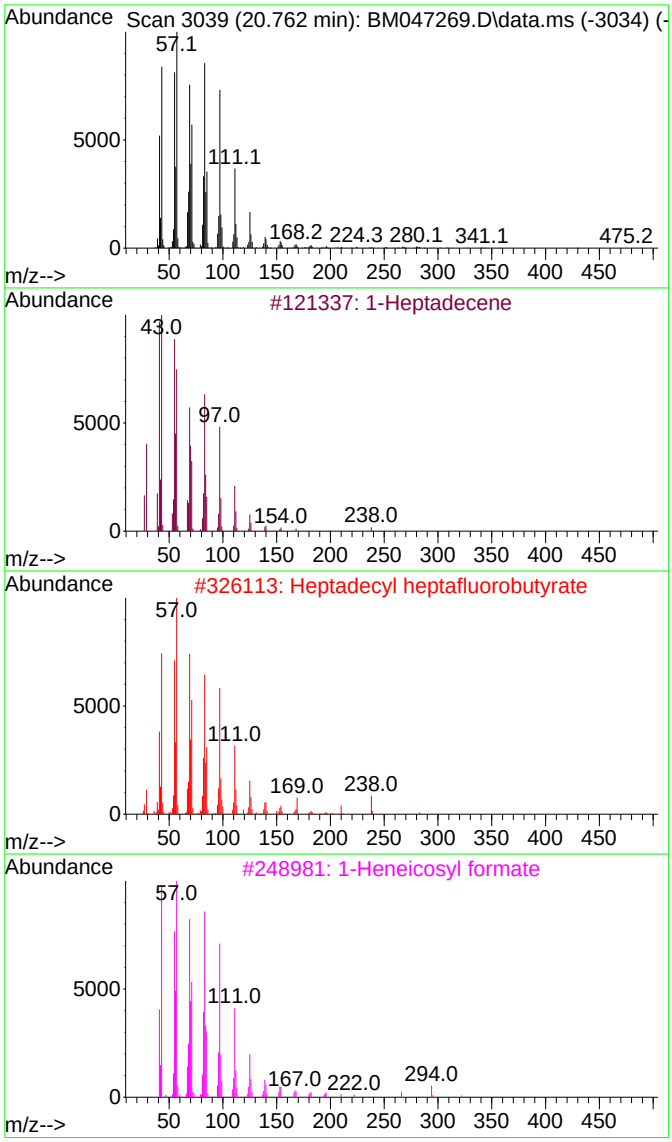
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

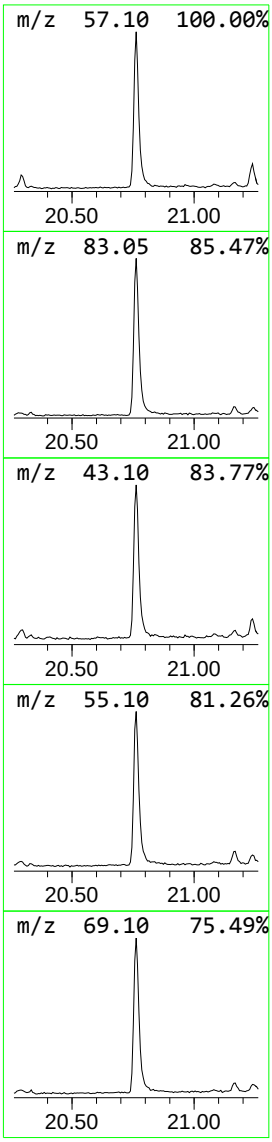
****

Peak Number 6 1-Heptadecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.762	10.92 ng	1737410	Chrysene-d12	21.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Cyclopentadecane	210	C15H30	000295-48-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047269.D
Acq On : 20 Aug 2024 13:27
Operator : RC/JU
Sample : P3643-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
932-K1-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.258	4.0	ng	238053	1	7.357	1197630	20.0
2-Pentanone, 4-...	4.569	5.4	ng	322813	1	7.357	1197630	20.0
1-Phenoxypropan...	10.875	3.9	ng	312336	2	10.116	1605580	20.0
n-Hexadecanoic ...	17.721	8.6	ng	1220240	4	16.786	2850710	20.0
Octadecanoic acid	19.021	3.8	ng	596555	5	21.027	3183440	20.0
1-Heptadecene	20.762	10.9	ng	1737410	5	21.027	3183440	20.0